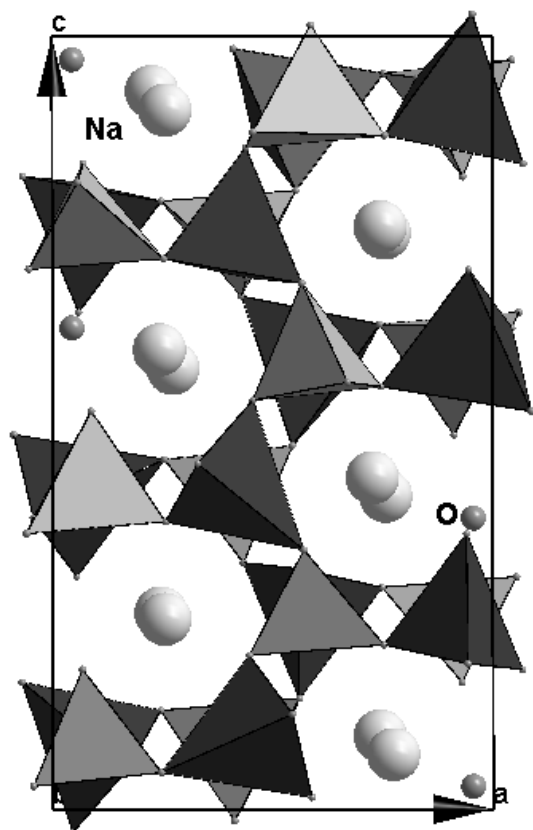


Crystal structure of sodium gallium germanium oxide, NaGaGeO₄

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Abstract

NaGaGeO₄, monoclinic, $P2_1/n$ (no. 14), $a = 8.8794(5)$ Å, $b = 8.2679(5)$ Å, $c = 15.5969(9)$ Å, $\beta = 90.129(5)^\circ$, $V = 1144.20$ Å³, $Z = 12$, $R(I) = 0.013$, $R(P) = 0.056$, $T = 293$ K.

Source of material

The NaGaGeO₄ sample material was prepared by mixing 10 mmol GeO₂, 5 mmol Ga₂O₃ and 5 mmol Na₂CO₃ in a ball mill for 15 minutes. This mixture was molten in a platinum crucible at 1200 °C for 24 h and subsequently quenched at room temperature. Crystallisation of the resulting glass was achieved by further heat treatment at 800 °C for 48 hours.

Experimental details

In the refinement the displacement parameters of the atoms and the framework atoms were constrained.

Discussion

NaGaGeO₄ crystallizes in space group $P12_1/n1$ as reported for the room temperature polytype by Barbier and Fleet [1]. The unit cell parameters obtained here are in good agreement with the values given in [1]. The structure is analogous to beryllonite (NaBePO₄) as given in ICSD file (no. 9271) [2], which provided the starting values for the refinement of the atomic coordinates. In the NaGaGeO₄ structure, GaO₂ (figure, light grey) and GeO₂ (dark grey) corner-sharing tetrahedra form a three-dimensional network with channel-like openings parallel to [010]. In these channels the sodium cations are regularly distributed.

Table 1. Data collection and handling.

Powder:	colorless, particle size < 63 µm
Wavelength:	Cu $K_{\alpha 1}, K_{\alpha 2}$ radiation (1.540596, 1.544493 Å)
μ :	186.45 cm ⁻¹
Diffractometer, scan mode:	Bruker AXS D8 Advance, Debye-Scherrer
$2\theta_{\max}$, stepwidth:	117°, 0.02
$N(\text{points})_{\text{measured}}$:	5351
$N(hkl)_{\text{measured}}$:	1628
$N(\text{parameter})_{\text{refined}}$:	80
Programs:	DIAMOND [3], TOPAS [4]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
Na(1)	4e	0.254(3)	−0.009(3)	0.247(3)	0.038(5)
Na(2)	4e	0.742(4)	0.434(4)	0.095(3)	0.038
Na(3)	4e	0.771(3)	0.022(4)	0.071(2)	0.038
Ge(1)	4e	0.920(2)	0.172(1)	0.2353(7)	0.014(2)
Ge(2)	4e	0.405(1)	0.172(2)	0.4227(7)	0.014
Ge(3)	4e	0.443(2)	0.164(2)	0.0897(7)	0.014
Ga(1)	4e	0.585(2)	0.280(1)	0.2661(7)	0.014
Ga(2)	4e	0.111(1)	0.273(2)	0.0836(8)	0.014
Ga(3)	4e	0.060(1)	0.270(1)	0.4075(8)	0.014
O(1)	4e	0.446(5)	0.264(4)	0.199(3)	0.014
O(2)	4e	0.066(5)	0.270(5)	0.181(3)	0.014
O(3)	4e	0.253(5)	0.255(6)	0.374(3)	0.014
O(4)	4e	0.749(5)	0.260(5)	0.215(3)	0.014
O(5)	4e	0.954(5)	0.233(5)	0.029(3)	0.014
O(6)	4e	0.589(4)	0.265(5)	0.015(3)	0.014
O(7)	4e	0.574(5)	0.176(4)	0.337(3)	0.014
O(8)	4e	0.250(5)	0.137(5)	0.047(3)	0.014
O(9)	4e	0.937(5)	0.151(4)	0.354(3)	0.014
O(10)	4e	0.559(4)	0.454(5)	0.312(2)	0.014
O(11)	4e	0.177(4)	0.456(6)	0.053(2)	0.014
O(12)	4e	−0.046(3)	0.464(5)	0.379(2)	0.014

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